Impurities in a Hubbard-chain

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Abstract. Using the density matrix renormalization group method we study the quantum coherence of one-dimensional interacting Fermi systems. We investigate the the effects of several kinds of impurities on the ground-state of a Hubbard chain in detail. Thereby we look at the transition from a metallic to an insulating ground-state caused by a local potential, a locally modified interaction or hopping. Unfortunately the preliminary results show that the successful treatment of a system of interacting spinless fermions, using the phase sensitivity as the observable of the phase transition, is unsuitable in the disordered Hubbard-chain. Nevertheless the data lead to new insight in the level structure. The investigation of the optical conductivity is still in progress. In addition we determine the exponent of the algebraic decay of Friedel oscillations at the boundary and around an impurity in the middle of the chain. These results are very useful for the characterization of the above mentioned impurities.

1 Introduction to the physical model

Disorder versus interaction induced metal-insulator-transition is a general question in solid state physics. The influence of electron-electron interaction on Anderson localization has attracted a lot of interest for several years. Hereby attention is also directed to randomly distorted one-dimensional systems, because the investigation of low dimensional systems can provide important insights. In contrast to higher dimensions, a detailed theoretical (analytical and numerical) description is possible in one dimension. In several cases analytical solutions are available; either exact, with the help of the Bethe-Ansatz, or approximative, using the bosonization technique. The latter is also suitable for distorted – hence non-integrable – systems. The density matrix renormalization group method [1] is a quasi-exact numerical method used to determine ground-state properties of long one-dimensional but non-integrable systems with excellent accuracy. Recent studies of a spinless fermion model have been a first step in a detailed understanding [2]. Whereas non-interacting fermions localize immediately in the presence of infinite small disorder in one dimension, a strong attractive interaction leads to a metal-insulator transition at a finite value of the disorder in this particular model. Special realizations of disorder, i. e. quasiperiodic potentials, likewise lead to a metal-insulator transition at finite value – even in the non-interacting case [3].

In this project we investigate the Hubbard model, the simplest model of interacting electrons with spin $\sigma = \uparrow, \downarrow$ on a chain. In the clean case, a Bethe-ansatz solution is known [4]. We consider $N_f = N_\uparrow + N_\downarrow$ electrons on a chain with length $L = Na$, where a is the lattice spacing,

$$H_{\text{Hubb}} = -\sum_{i,\sigma}^{N} t_i \left(c^+_{i,\sigma} c_{i+1,\sigma} + \text{h. c.}\right) + \sum_{i}^{N} U_i n_{i,\uparrow} n_{i,\downarrow} + \sum_{i}^{N} \epsilon_i n_i, \qquad (1)$$

where the operators $c^+_{i,\sigma}$, $c_{i,\sigma}$, $n_{i,\sigma}$, and $n_i = [n_{i,\sigma} + n_{i,\sigma}]/2$ denote Fermi creation, annihilation and number operators. The magnetization is given $M = N_\uparrow - N_\downarrow$. Disorder can be introduced by local potentials of random strength, $\epsilon_i\ \epsilon[-W/2; W/2]$, randomly distributed $U_i\ \epsilon[-W/2i + U; W/2 + U]$, or $t_i\ \epsilon[-t - W/2; -tW/2]$. Initially we consider single impurities, given by a local potential at site n, $\epsilon_i = \delta_{in}\epsilon_n$, a locally modified interaction, $U_i = U(1 - \delta_{in}u)$, and tow symmetric modified bonds, $t_i = t(1 - \delta_{in}b - \delta_{in+1}b)$.

The clean model ($W = 0$) shows three phases. Phase one appears for $U < 0$, where the spin-excitation spectrum has a gap and the the low-lying charge-excitations can be described by those of a Luttinger liquid [5]. Phase two for $U \geq 0$ and away from half filling, is characterized by gapless spin- and charge-excitations. The last phase occurs for $U > 0$ and half filling, where the charge excitations have a gap and the spin-excitations are those of a Luttinger liquid.

In the previous studies of an equivalent model for interacting spinless fermions in periodic, quasiperiodic and random potentials [2,3,6], the metal-insulator transition was determined with the help of the phase sensitivity, $N\Delta E = [E(\pi) - E(0)]$, [7], i.e. the energy difference between periodic, $E(\Phi = 0)$, and anti-periodic boundary conditions, $E(\Phi = \pi)$. The different boundary condition are modeled via a magnetic flux enclosed in the ring, $c_{i+L} = \exp(i\Phi)c_i$. In a metal, exact solutions based on the Bethe-ansatz or conformal field theory show that this energy difference decreases with $1/N$. Thus the phase sensitivity is constant in this case. In an insulator, on the other hand, the system cannot react to the twist in the boundary condition, i.e. the phase sensitivity is expected to decrease with system size.

The situation is more complicated in the Hubbard-model. The phase sensitivities for up- and down-spins can be related to the spin- and charge-stiffness, see [7]. By considering again periodic and anti-periodic boundary conditions for the spin-up and spin-down electrons, we can write

$$E(\Phi_\uparrow, \Phi_\downarrow) = \frac{D_c}{2}[2\pi(J_\uparrow + J\downarrow) + (\Phi_\uparrow + \Phi_\downarrow)]^2 + \frac{D_s}{2}[2\pi(J_\uparrow - J\downarrow) + (\Phi_\uparrow - \Phi_\downarrow)]^2, \qquad (2)$$

where the $J_{\uparrow,\downarrow}$ are the quantum numbers of the topological excitations. Evaluating the above formula, we find

$$E(\pi,0) - E(0,0) = \frac{\pi^2}{2}(D_c + D_s^E) \tag{3}$$

$$E(\pi,\pi) - E(0,0) = 2\pi^2 \min(D_c, D_s^E). \tag{4}$$

The spin-stiffness D_s can also be obtained – in the clean system away from half filling and $U \geq 0$, i. e. in the Luttinger liquid phase – from the energy difference between the ground-state energy for different magnetizations,

$$E(N, N_f, M) - E(N, N_f, M-1) = 2\pi^2 D_s^{\Delta}/N. \tag{5}$$

In the case of attractive interaction, this energy difference gives, together with a finite size scaling, the gap in the spin excitations. The identity $D_s^E = D_s^{\Delta}$ was checked numerically with reasonable accuracy. In addition the numerical values of D_c and D_s are correctly produced for the clean system. As far as these tests are concerned, the phase sensitivities seems again to be a suitable observable.

For the study of the disordered Hubbard-chain, we need to compute the ground-state energy very accurately for different boundary conditions, long system sizes and, in addition, for different fillings. Since numerical methods like exact diagonalization (ED) and quantum Monte Carlo (QMC) simulations are restricted either to small systems or to finite temperatures, we use the density matrix renormalization group technique (DMRG) [1].

To complete the investigations of the disordered Hubbard-chain we calculate the Friedel oscillations at the boundary and around an impurity in the middle of the chain. In the case of $N_\uparrow \neq N_\downarrow$ they were already determined, [8]. We therefore consider the case $N_\uparrow = N_\downarrow$. In this case, logarithmic corrections are expected. Using conformal field theory, the local behavior of the density at a boundary is given by the density-density-correlation-function [9]. The Friedel oscillations are then given by [10]

$$n(x) - n_0 \propto \frac{\cos(2k_F x)}{x^{(1+g_c)/2} \ln^{3/4} x}, \tag{6}$$

where $g_c(U) \approx 1 - U/(2t\pi)$ is the Luttinger-parameter.

2 The density matrix renormalization group method

2.1 Numerical and Computational Aspects

The DMRG is an improvement of the blocking scheme of the numerical real space renormalization treatment (NRG) [11]. The method is used to determine the ground-state properties of long systems (about a hundred lattice sites, compared to about thirty using ED). The complete lattice is ithereby

built up out of smaller subsystems A, B – by considering in each step only the m states of the subsystems which contribute mostly to the ground-state, $|\Psi_C\rangle = \sum_{ij} c_{ij} |\psi_i^A\rangle |\psi_j^B\rangle$, of the whole system C. This most important states are gained in the DMRG with the help of the density matrix. The dimension of the new Hamilton matrix in the NRG is in contrast reduced by considering only the m states with the lowest energy. Thus each step of the algorithm works as follows: Starting with a system of length M, one site is added – this system is called A. C is built from A and $B = A$. Now the ground-state of C and the coefficients c_{ij} are calculated by diagonalizing the Hamilton matrix using the Davidson algorithm for sparse matrix diagonalization [12]. The density matrix, $\rho_= \sum_j c_{ij} c_{mj}^*$, a fully occupied matrix, is diagonalized using standard library (ESSL) routines. Finally all states and operators have to be transformed to the new basis which consists of the m states corresponding to the m lowest eigenvalues of the density matrix. For the implementation, see [13]. The number of states which have to be kept for reasonable accuracy (about 10^{-4}) depends mostly on the boundary conditions and the criticality of the system. We typically kept $m = 200 \ldots 400$ states in the calculations of the disordered system where the system sizes varied from $N = 30 \ldots 60$. The demands on the memory lay in the region of about 500-1000 MB. In the finite lattice algorithm all states and operators for all sizes of the intermediate subsystems must be stored. Thus, we need about 100 MB temporary disk space.

2.2 Vectorization, Parallelization and Performance

According to several symmetries of the Hamiltonian and conserved quantities – such as the fermion number or the magnetization – the block structure of the Hamilton matrix is used to save space and time. For this reason the blocks are relatively small (about 500×500) and the program was optimized for a serial processor and run on the IBM/RS6000 SP. The code was written in C++. The program spend most of the time in the subroutine where the Hamiltonian is diagonalized. Hence, the Davidson algorithm has to be optimized. It was possible to reach a performance of about 100-200 Mflops on a single processor. Parallelization (using MPI) was mostly carried out to obtain the results for various parameters in a reasonable time.

3 Results for the metal-insulator transition in a Hubbard-chain

As mentioned above, we start our studies of disordered systems by considering only one impurity. In this case the averaging over many disorder configurations can be omitted. Furthermore, the renormalization group (RG) treatment of [14] can be used to check the numerical data. The most important result is that even a weak impurity destroys the structure of the energy-levels with the external flux.

3.1 A local potential

The RG treatment for a local potential shows that the local potential leads to insulating behavior (decrease of the phase sensitivity or stiffness with system size) for all fillings, impurity strengths and interactions.

In Fig. 1 we show the numerical results for a local potential at half and third filling ($\rho = N_f/N$). We begin by discussing the left hand side of Fig 1. At half filling the Hubbard-model is symmetric in spin and charge. $N[E(\pi,\pi) - E(0,0)]$ shows for weak impurity strength the expected symmetric behavior for $U > 0$ and $U < 0$ (spin-gap versus charge-gap behavior) and a decrease of the phase sensitivity with system length. But this decrease is clearly related to the localization due to the interaction, U. The overall decrease of the phase sensitivity is due to the impurity. A local potential couples spin and charge. Thus this symmetry vanishes by adding the impurity. In our case we find a small increase near $U = 0.5t$ which was already found by [15]. This maximum is shifted to $U = 1t$ for stronger impurity strength. The same behavior is found for $N[E(\pi,0) - E(0,0)]$, where the unexpected (wrong?)

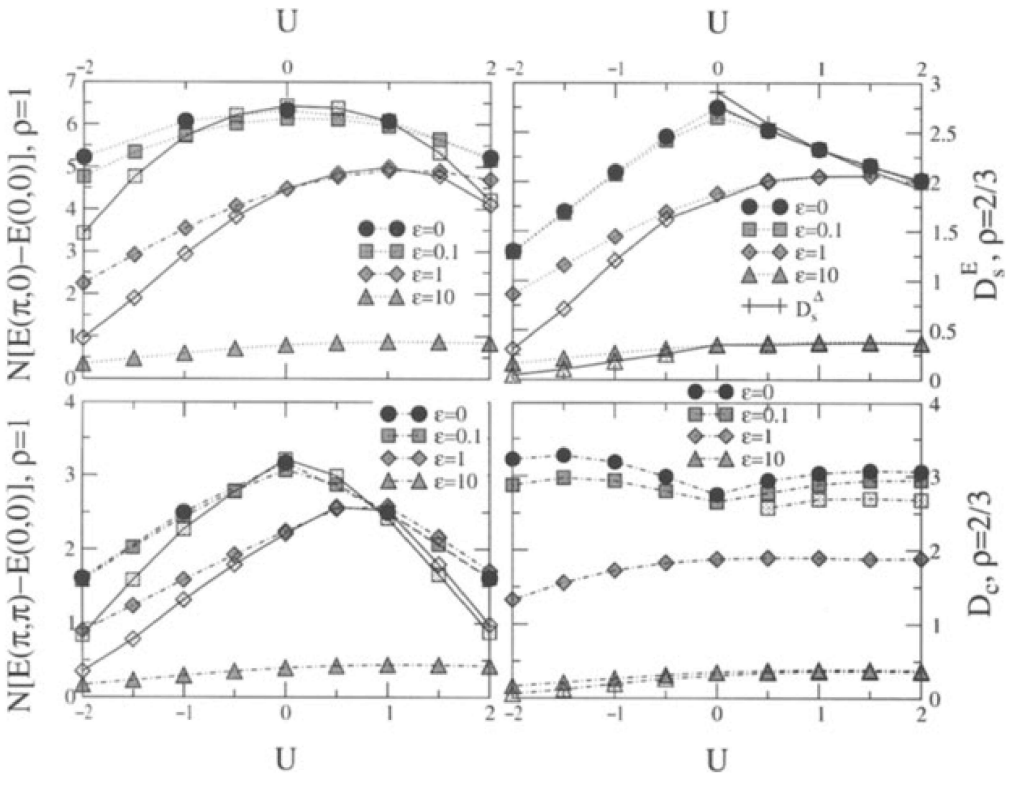

Fig. 1. Phase sensitivity or extracted stiffness versus interaction for a Hubbard-chain with a local potential. On the left side we show the results for half filling, on the right for third filling, respectively. The circles denote the clean systems at $N = 10$ or $N = 9$, respectively. The squares denote an impurity of strength $\epsilon_1 = 0.1t$, the diamonds an impurity of strength $\epsilon_1 = 1t$, and the triangles an impurity of strength $\epsilon_1 = 10t$. The dark shaded symbols correspond to $N = 10$ or $N = 9$, respectively, and the light shaded symbols to $N = 30$ or $N = 27$.

metallic behavior is between $-0.5t < U < 1t$ for small impurity strength and between $0t < U < 1t$ for stronger. The assignment of the phase sensitivities to the spin- and charge-stiffness for the whole interaction regime is possiblei for third filling. The spin-stiffness, to be more precise D_S^E, shows partly the expected behavior: A clear decrease with system size for $U < 0$ in the spin-gap-phase is seen. From the renormalization group treatmenti, however, we also expect a decrease of the spin-stiffness with system length due to the impurity for repulsive interaction. This is not found in the numerical data. In addition the spin-stiffness deduced from the spin-gap (marked with a + in the upper right corner of Fig. 1) is completely independent of the impurity strength. Thus it is not possible to make a statement of a possible transition in the spin-sector with help of the phase sensitivity. As far as the charge stiffness is concerned, we find at least the decrease for small impurity strength and repulsive interactions.

3.2 Locally modified interaction

The numerical studies of a system with a modified interaction $U_i = U' = U(1-u)$ at the impurity site and $U_i = U$ otherwise lead to no significant results as in the case of the local potential. This impurity type should show a metal-insulator transition as a function of the impurity strength. Whereas the system is supposed by the bosonization treatment to stay metallic for small impurity strength, $u \ll 1$, it should become insulating either for $U' \ll U$ and $U' \gg U$, where the impurity can be considered as a local, spin-dependent potential. The numerical data are shown in Fig. 2. It is not possible to extract the metal-insulator transition from this data. Obviously this impurity enhances the spin-gap for $U < 0$, where we find a very sharp decrease. Another result worth mentioning is that in this case D_s^Δ depends strongly on the impurity strength, whereas D_s^E is only weakly dependent on it. In particular we see that the ground-state energy for $M \neq 0$ does not depend on the impurity strength for all boundary conditions. For $M = 0$, on the other hand, the ground-state energy is a monotonic decreasing function with U for $U' \ll U$ as for $U' = U$. In the contrary limit, $U' \gg U$ the ground-state energy increases with U for attractive interactions, but decreases for repulsive.

3.3 Two symmetric modified bonds

In this case we find for the non-interacting system that the backscattering contributions from this impurity cancel out for half filling in first order, and are reduced for third filling.

The numerical data shown in Fig. 3, show clearly the slight reduction of the phase sensitivity for weak impurities for half filling at fixed chain length. Stronger impurities lead to a larger decrease which is, in addition, strengthened by increasing repulsive interaction. In the case of third filling, D_S^E is – due to the incomplete cancellation of the backscattering – distinctly reduced

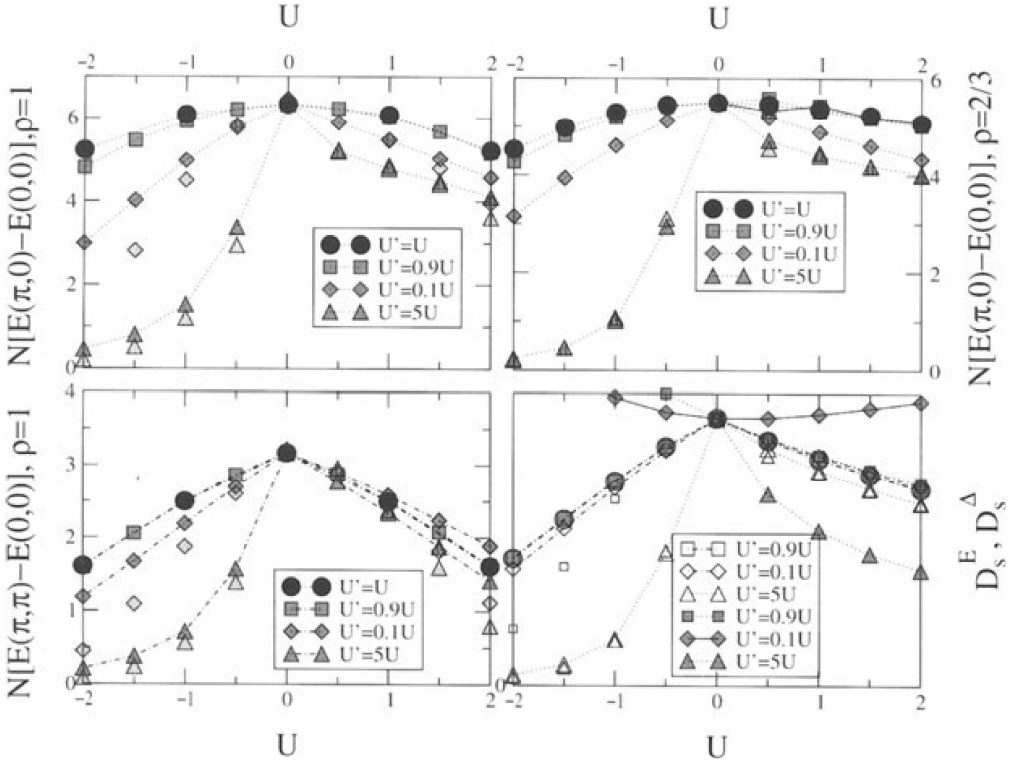

Fig. 2. Phase sensitivity or extracted stiffness versus interaction for a Hubbard-chain with a modified interaction. On the left side we show the results for half filling, on the right for third filling, respectively. The circles denote the clean systems at $N = 10$ or $N = 9$, respectively. The squares denote an impurity of strength $U' = 0.9U_0$, the diamonds an impurity of strength $U' = 0.1U_0$, and the triangles one of strength $U' = 5U_0$. The dark shaded symbol correspond to $N = 10$ or $N = 9$, respectively, and the light shaded symbols to $N = 30$ or $N = 27$. In the lower right plot D_s^E is marked with the open symbols and D_s^Δ with shaded symbols.

in the non-interacting system. Increasing the interaction the localizing effects of the impurity are weakened. The behavior of D_s^Δ is complementary. The identity $D_s^E = D_s^\Delta$ holds above a critical interaction, $U_c = 5b$.

4 Friedel-oscillations

In Fig. 4 we show results for the decay of the Friedel oscillations at the boundary. In this case, for half filling, an algebraic decay rather than the pronounced algebraic decay with logarithmic corrections is found. Nevertheless, the exponents obtained from the numerical data are not in agreement with the predictions from bosonization. The data for third filling show no clear behavior.

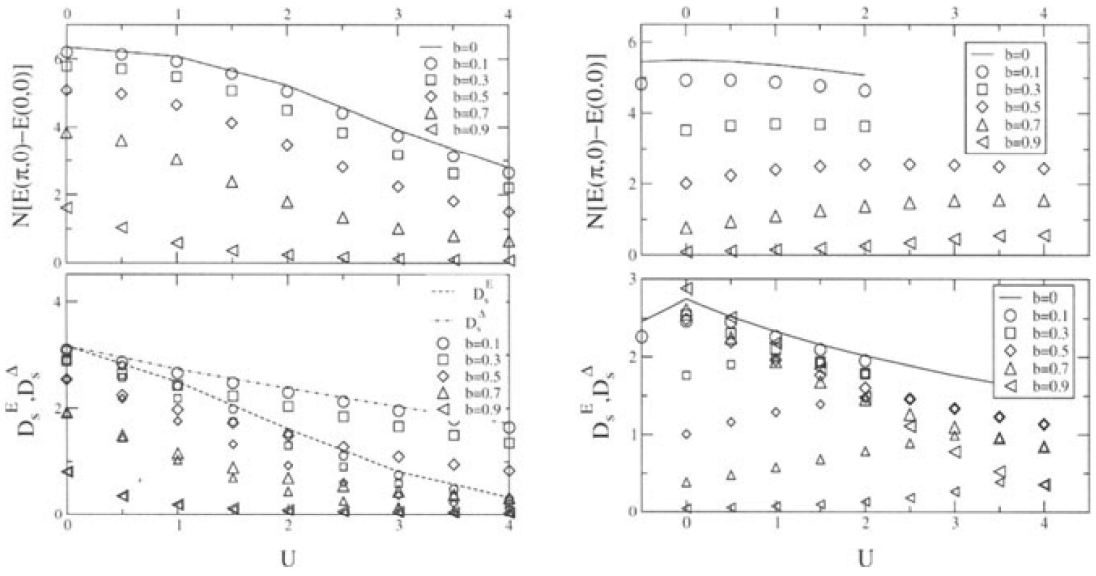

Fig. 3. Phase sensitivity or extracted stiffness versus interaction. On the left side we show the results for half filling, on the right side for third filling, respectively. The system length is $N = 10$ for half filling and $N = 9$ for third filling. In the lower panel, the larger symbols correspond to D_s^{Δ}, the smaller to D_s^{E}.

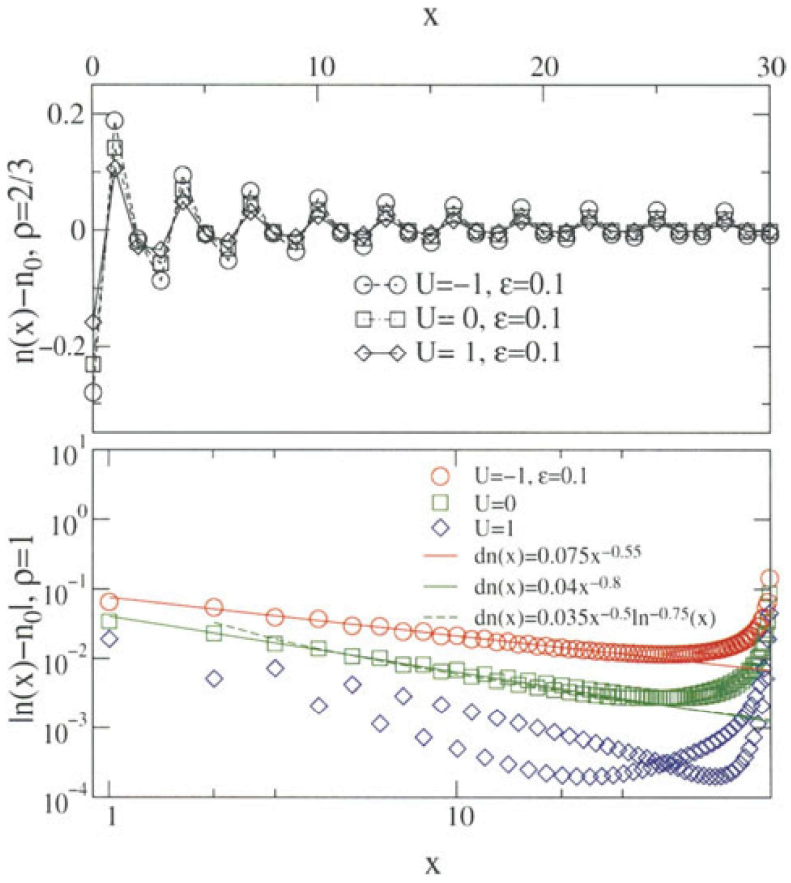

Fig. 4. Local density-distribution versus distance for half and third filling and $U = -1, 0, 1$. An additional potential scatterer is located at the ends of the chain, $\epsilon_1 = \epsilon$, $\epsilon_N = -\epsilon$. In the upper plot, the lines are connecting the data points.

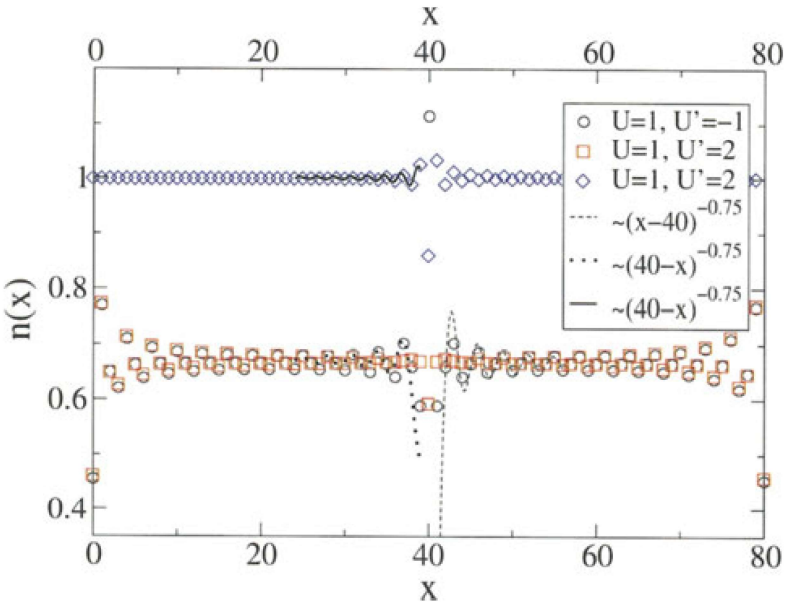

Fig. 5. Local density-distribution versus distance for half and third filling and $U = 1$. The interaction in the middle of the chain is modified, $U' = -U$ or $U' = 2U$.

They can be described either with or without logarithmic corrections. For example we find,

$$\begin{aligned} n(x) - \rho &= -0.35\cos(\rho\pi x + 0.85)x^{-0.5}\log^{-0.75}(x) \quad U = -1 \\ &= -0.6\cos(\rho\pi x + 0.85)x^{-1}\log^{-0.75}(x) \quad U = 0 \\ &= -0.25\cos(\rho\pi x + 0.85)x^{-0.75}\log^{-0.75}(x) \quad U = 1. \end{aligned}$$

Considering the logarithmic corrections, the exponents agree well with the predictions from bosonization. The prefactor depends only weakly on the additional local potential, as was found in the case of $N_\uparrow \neq N_\downarrow$ using the Bethe-ansatz, [8]. Fig. 5 shows the results for the decay around an impurity which is given by a modified interaction in the middle of the chain. Again, we find oscillations at the boundary, now without an additional potential. The decay around the impurity in the middle of the chain shows the logarithmic corrections more clearly.

5 Summary and outlook

Contrary to the model of spinless fermions on a ring, where it was possible to characterize the metallic and insulating phases as well for different kinds of impurities as well as for random, quasi-periodic and periodic potentials, the phase sensitivity is not a suitable observable in the Hubbard model. The second degree of freedom in the Hubbard model changes most features essentially. Only the case of two modified bonds is comparable in both systems. To overcome these problems concerning the level structure, we try to gain reasonable results using the optical conductivity. As reported in [16], the Drude

weight which corresponds to our phase sensitivity can be determined easily by calculating the real part of the optical conductivity using open boundary conditions. In this case a precursor of the Drude peak is seen for small energy transfer for open boundaries. It is possible [17] to calculate the optical conductivity with the DMRG technique by targeting not only the ground-state but the lowest excitations and then using the Lanczos technique. Effects of the open boundaries are smoothed by a filter function. Nevertheless, preliminary studies of the system containing a single impurity using exact diagonalization show that this additional, indeed very sharp peak, does not disappear even for strong impurities. Further investigations have to show whether the optical conductivity is a better choice to determine the transition from the metal to the insulator. A second project concerned the local density and magnetization. In the last years, many new materials have been synthesized, but in some cases the theoretical description is yet not found. Studying the local behavior, possibly the relevant theoretical model can be identified. We found that the logarithmic corrections occur in the case of a bulk impurity but are maybe absent in the case of the decay near a boundary at the open end of the chain. Thus, further investigations are necessary.

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